N-Cycloheptyl-N'-phenylurea 19095-79-5 | DTXSID10172606

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 5.85e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.78e-01

Confidence level: 3.15e-01

Nearest Neighbors from the Training Set

Image not found

2-Propanone, 1,3-diphenyl-

Measured: 7.53e-06 Predicted: 3.07e-04

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Hydroprene

Measured: 3.39e-09 Predicted: 8.80e-04

Image not found

Phenyl glycidyl ether Measured: 4.36e-04 Predicted: 1.23e-02

Image not found

Ethylenediaminetetraacetic acid

Measured: 1.40e-06 Predicted: 2.81e-12